||| 1.0

||| 2.8 ||| 2.5

||| 3.2

||| 2.2

||| 3.6

||| 4.0 ||| 2.0

||| 1.1

||| 1.8

||| 1.25 ||| 1.4 ||| 1.6

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SIMULATING A MARKOV CHAIN WITH A

SUPEREFFICIENT SAMPLING METHOD

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Abstract

This paper describes an algorithm and a FORTRAN subprogram, CHAIN,
for simulating the behavior of an $(n+1)$ state Markov chain using a
variance reducing technique called *rotation sampling*. The simulation of
k *microreplications* is carried out in parallel at a mean cost $\leq O(\ln k)$
and with variances of sample quantities of interest $\leq O((\ln k)^2/k^2)$.
The program allows for independent *macroreplications*, each of k micro-
replications, in order to facilitate estimation of the variances of sample
quantities of interest. The paper describes theoretical results that
underlie the algorithm and program in Section 1 and presents applications
of interest for first passage time and steady-state distributions in
Section 2. Section 3 describes the algorithm and CHAIN and an example
in Section 4 illustrates how CHAIN works in practice. Section 5 describes
the options available for restarting the simulation.

- B -

Introduction

A recent paper (Fishman 1981) describes how one can use rotation sampling, a special case of the antithetic variate method, to induce substantial variance reduction in the simulation of a finite state Markov chain. Since many discrete event simulations have an underlying Markov structure or one close to being Markov, this variance reducing proposal has clear appeal. Moreover, for large and possible ill-conditioned transition matrices, one may prefer the Monte Carlo or simulation method with appropriate variance reducing plans to numerical analysis when solving for steady-state and first passage time distributions. In fact, it may be the only feasible method for some problems.

This earlier work derives its cost-saving potential from viewing the simulation of k tours in *series* of a finite $(n+1)$ state positive recurrent aperiodic Markov chain as equivalent to the simulation of k replications of the Markov chain in *parallel*. Although the marginal distributions that arise with the two alternative formulations are necessarily the same for corresponding variables, the parallel formulation alllows one to induce joint distributions across replications that lead to a significant cost saving. The induced joint distributions follow from the use of rotation sampling, as described in detail in Fishman and Huang (1980). The cost saving arises in two ways. Firstly, for fixed n, run time in the correlated case is $O(\ln k)$ in contrast to $O(k)$ for the serial simulation. Secondly, for fixed n the

variance of an estimator of interest has an upper bound $O((\ln k/k)^2)$ for the correlated case compared to $O(1/k)$ for the serial case.

The present paper describes an algorithm for implementing the essential steps for k parallel simulations with correlation along individual sample paths induced by rotation sampling. The paper also describes a FORTRAN program, called CHAIN, that one can use to perform the simulation. In particular, CHAIN runs I independent *macroreplications* each of K correlated parallel *microreplications* and computes point estimates of interest and sample variances of these point estimates.

Section 1 introduces the Markov chain rotation and describes the results on variance reduction derived in Fishman (1981a) for finite state chains. For completeness it also presents results in Fishman (1981b) for infinite state chains. Section 2 describes several potential uses of CHAIN. These include first passage time distributions and steady-state probabilities for semi-Markov processes. Section 3 presents Procedure MC which contains the essential steps in carrying out parallel simulation based on rotation sampling. It also describes the FORTRAN CHAIN subprogram in detail. Section 4 describes an example of how CHAIN can be used in practice. The example is of the discrete time Markov chain that corresponds to the M/M/1 queueing problem with finite capacity n .

1. Definitions and Previous Results

Consider a positive recurrent aperiodic Markov chain with state space $S = (0,1,2,\ldots,n)$ and transition probabilities $\{p_{ij}; i,j=0,1,\ldots,n\}$

where there exists a positive integer $\delta \leq (n-1)/2$ such that

$$p_{ij} = 0 \qquad\qquad \text{for } |i-j| > \delta$$

and   (1)

$$\sum_{j=\max(0,i-\delta)}^{i+\delta} p_{ij} = 1 \quad .$$

It is convenient to describe an alternative, but equivalent, representation
to (1) whose value is apparent when actually generating sample paths by
simulation on a computer. Let s_j denote the total number of states that
have positive transition probabilities from state j and let
$\{m_{jr}; r = 1,\ldots,s_j\}$ denote the ordered sequence $(m_{jr} < m_{j,r+1}; r = 1,\ldots,s_j - 1)$
of the s_j states to which entry can occur from state j . Then one has the
representation

$$p_{jm_{jr}} > 0 \qquad\qquad r = 1,\ldots,s_j$$

$$\sum_{r=1}^{s_j} p_{jm_{jr}} = 1$$

$$\delta \geq \max \left(|m_{j1} - j| , |m_{js_j} - j| \right) \qquad j = 0,1,\ldots \quad .$$

Suppose one wants to use simulation to study the behavior of the chain during a time period that begins with exit from state a and ends with entry to state $b \in S$. Consider k replications of the simulation experiment run in parallel. Let $K'_{ij\ell}$ denote the number of replications that move from i to j on transition ℓ and let $K'_{j\ell}$ be the number of replications in state j at the end of transition ℓ.[†] Let $U, U_1, \ldots, U_{K'_{j\ell}}$ be from $U(0,1)$ where $K'_{j\ell} > 0$ is given. Then for parallel replications one can represent $K'_{jm_{jr}\ell+1}$ as

$$K'_{jm_{jr}\ell+1} = \sum_{m=1}^{K'_{j\ell}} I_{[q_{j,r-1}, q_{jr})}(U_m) \qquad (2)$$

where

$$q_{j0} = 0$$

$$q_{jw} = \sum_{r=1}^{w} p_{jm_{jr}} \qquad w=1,\ldots,s_j; \; j=0,1,\ldots$$

and

$$I_{[u,v)}(x) = 1 \qquad u \le x < v$$
$$= 0 \qquad \text{otherwise.}$$

To ensure that each replication begins with an exit from state a and ends with the first entry into state b, one replaces the original $\{p_{bj}; j=1,\ldots,s_b\}$ by $p_{bb} = 1$ and sets $p_{bm_{br}} = 0$ for

[†] The prime superscript is used here for consistency with the notation in Fishman (1981a, 1981b). However, without loss of generality, we take the initial state here as a and the final state as b whereas in the earlier work the initial and final states were 0 and a respectively. This relabeling of initial and final states makes the generality of the approach more apparent to the reader.

$r = 1,\ldots,s_b$ and $r \neq b$. If $b = a$, these modifications are made after the first transition.

If one uses the *rotation sampling plan*

$$U_m = U + \frac{m-1}{K'_{j\ell}} \qquad\qquad 0 \leq U < 1 - \frac{m-1}{K'_{j\ell}}$$

$$\tag{3}$$

$$= U + \frac{m-1}{K'_{j\ell}} - 1 \qquad\qquad 1 - \frac{m-1}{K'_{j\ell}} \leq U < 1 ,$$

then the results in Fishman (1981a,b) apply. In particular,

$$\text{var } K'_{ij\ell} \leq 0(1) \tag{4}$$

and for $S_b = S - b$, the sample number of transitions from i to j is

$$R'_{ijk} = \sum_{\ell=1}^{\infty} K'_{ij\ell} \tag{5a}$$

and the sample mean reward is

$$R'_k = \frac{1}{k} \sum_{\ell=1}^{\infty} \sum_{i \in S_b} \sum_{j \in S} A_{ij} K'_{ij\ell} . \tag{5b}$$

Then one has

$$\text{var } R'_{ijk} \leq 0((\ln k)^2) \tag{5c}$$

and, if $|A_{ij}| \leq 0(1)$,

$$k^2 \text{ var } R'_k \leq 0(\delta^2 (\ln k)^4) \qquad \text{as } n \to \infty \tag{5d}$$

$$k^2 \text{ var } R'_k \leq 0((n\delta \ln k)^2) \qquad n < \infty.$$

Here we speak of $\{A_{ij}\}$ as the reward function. Finally, the number of steps to total absorption

$$T'_k = \min(t: K'_{bt} = k)$$

has

$$E\ T'_k = O(\ln k)$$

and

$$\text{var}\ T'_k \leq O((\ln k)^2)\ .$$

(6)

Note that the sampling scheme (3), when used in (2), preserves the identical and correct probability laws along the sample paths of each of the k replications. An equivalent expression for $K'_{jm_{jr}\ell+1}$, which leads to a computational saving, is:

$$K'_{jm_{jr}\ell+1} = \lfloor Q \rfloor - \lfloor P \rfloor + I_{[\overline{P},\overline{Q})}(\overline{K'_{j\ell}U}) \qquad \overline{P} \leq \overline{Q}$$

(7)

$$= \lfloor Q \rfloor - \lfloor P \rfloor - I_{[\overline{Q},\overline{P})}(\overline{K'_{j\ell}U}) \qquad \overline{P} > \overline{Q}$$

where

$$P = K'_{j\ell}\ q_{j,r-1},$$

$$Q = K'_{j\ell}\ q_{jr}$$

and $\bar{x} = x - \lfloor x \rfloor$. Here the cost of sampling the transitions from state j based on (7), and using the inverse transform method, is $C(s_j) \leq 0(2\delta + 1)$ and independent of k whereas sampling cost based on (2) is at best $0(k)$.

Let S_k' denote the cost of simulating (1) using (3) in (7). For a countably infinite state space, no more than $(2\delta + 1)\ell$ transient states are occupied prior to transition $\ell+1$ and, therefore, no more than $(2\delta + 1)(\ell^2 + \ell)/2$ sampling events occur through transition ℓ . Since each (i,j) transition has cost $0(2\delta + 1)$, one has $S_k' \leq 0((\delta T_k')^2)$ so that

$$E \, S_k' \leq 0((\delta \ln k)^2) . \tag{8a}$$

For the finite state case

$$E \, S_k' \leq 0(n \, \delta \ln k) . \tag{8b}$$

These results compare favorably with the case of independent replications taken in series where R_{ijk} and R_k , the sample number of transitions from i to j and the sample mean reward, respectively, have $\text{var} \, R_{ijk} = 0(k)$ and $k \, \text{var} \, R_k = 0(1)$. Moreover, for simulation cost S_k , one has $0(k) \leq E \, S_k \leq 0(\delta k)$. The lower bound arises when n is small enough to allow storage of all distributions and their *aliases* required by the alias method (Walker 1977) to determine the entered state from each existing state at each transition. The upper bound arises from use of the inverse transform method to determine the paths. See Fishman (1981b) for a more detailed discussion of this cost.

It is also noteworthy that the desirability of k parallel replications with rotation sampling relative to a simulation of k independent replications in series continues to hold when $\{A_{ij}\}$ is not bounded, provided that $\operatorname{var}(A_{ij} K'_{ij,\ell+1} | K'_{i\ell}) < \infty$.

2. Potential Uses

This section describes three uses to which the previously described rotation sampling plan can be put with regard to estimation.

First Passage Times

Let

h_ℓ = probability of moving from state a to state b for the

first time in exactly ℓ steps

and   (9)

$$H_\ell = \sum_{i=1}^{\ell} h_i = \text{probability of moving from state } a \text{ to state}$$
b for the first time in no more than ℓ steps.

As estimators of h_ℓ and H_ℓ one has, respectively,

$$\hat{h}_\ell = \frac{1}{k} \sum_{j \in S_b} K'_{jb\ell} = \frac{1}{k} (K'_{b\ell} - K'_{b,\ell-1}) \qquad K'_{b0} = 0$$

                                                                                             (10)

and

$$\hat{H}_\ell = \frac{1}{k} \sum_{i=1}^{\ell} \sum_{j \in S_b} K'_{jbi} \qquad\qquad \ell = 1,2,\ldots \; .$$

Let $S'_{k\ell}$ denote the cost of simulating (1) up to and including step using the rotation sampling plan (3) with (7). Theorem 1 gives several relevant properties for $\hat{h}_\ell$, $\hat{H}_\ell$ and $S'_{k\ell}$.

__Theorem 1.__   For a simulation of k parallel replications of (1) using (3) and (7) one has:

  (i) $E \hat{h}_\ell = h_\ell$.

  (ii) $E \hat{H}_\ell = H_\ell$.

  (iii) $\text{var } \hat{h}_\ell \leq O((\varepsilon/k)^2)$.

  (iv) $\text{var } \hat{H}_\ell \leq O((\delta\ell/k)^2)$.

  (v) $E S'_{k\ell} \leq O((\delta\ell)^2)$.

__Proof.__   Since the correct probability law continues to prevail on sample paths for each replication, one has $E K'_{jb\ell} = k h_\ell$ so that (i) and (ii) follow immediately. Since $\text{var } K'_{jb\ell} \leq O(1)$ and no more than 2δ states can transit to state b , it is clear that

$$\text{var}(\textstyle\sum_{j \in S_b} K'_{jb\ell}) \leq O(\delta^2)$$

and that (iii) holds. Since there are exactly ℓ steps to consider, (iv) follows immediately. Here $\hat{H}_\ell$ is a special case of (5b) with $A_{ib} = 1$ $i \in S_b$ and $A_{ij} = 0$ otherwise. Since exactly ℓ steps occur no more than $(2\delta + 1)(\ell^2 + \ell)/2$ trials are necessary each with cost $O(\delta)$. Therefore, (v) obtains.

   If one were to perform k independent replications in series, then $\text{var } \hat{h}_\ell = O(1/k)$, $\text{var } \hat{H}_\ell = O(\ell^2/k)$ and $E S_k \geq O(k)$, emphasizing the benefit of rotation sampling plan (3) and the conciseness of (7).

Steady-State Distribution

Let

p_j = probability of being in state j at an arbitrarily selected

time $j = 0,1,\ldots,n$.

As an estimator of p_j one has

$$\hat{p}_j = G_{jk}/G_k \tag{11}$$

where

$$G_{jk} = \frac{1}{k} \sum_{t=1}^{\infty} \sum_{i=0}^{n} K'_{ijt} \qquad\qquad j=0,1,\ldots,n$$

and

$$\tag{12}$$

$$G_k = \sum_{j=0}^{n} G_{jk} \ .$$

Since $\hat{p}_j$ is a *ratio* estimator it has bias

$$E(\hat{p}_j - p_j) \doteq p_j^2 \left[\frac{\operatorname{var} G_k}{E^2 G_k} - \frac{\operatorname{cov}(G_{jk}, G_k)}{E\,G_{jk} \cdot E\,G_k} \right] \tag{13}$$

and variance

$$\operatorname{var} \hat{p}_j \doteq p_j^2 \left[\frac{\operatorname{var} G_k}{E^2\,G_k} - \frac{2\,\operatorname{cov}(G_{jk},G_k)}{E\,G_{jk} \cdot E\,G_k} + \frac{\operatorname{var} G_{jk}}{E^2\,G_{jk}} \right] \ . \tag{14}$$

From the results of Section 1, one has

$$\text{var } G_{jk} \leq O((\delta \ln k/k)^2) \quad \text{and} \quad \text{var } G_k \leq O((n \ln k/k)^2)$$

so that both bias and variance benefit from rotation sampling.

Steady-State Probabilities for a Semi-Markov Process

The results presented so far relate directly to a Markov chain.
However, their extension to semi-Markov processes is relatively direct
for the steady-state probabilities. Let μ_{ij} denote the mean time spent
in state i prior to transiting to state j. For the steady-state prob-
abilities, one now has the estimators

$$\tilde{p}_j = G'_{jk}/G'_k \qquad\qquad j=0,\ldots,n$$

where

$$G'_{jk} = \sum_{t=1}^{\infty} \sum_{i=0}^{n} \mu_{ij} K'_{ijt}$$

and

$$G'_k = \sum_{j=0}^{n} G'_{jk} \quad .$$

Then $\tilde{p}_j$ has approximate bias and variance as in (13) and (14), respectively,
with G'_{jk} replacing G_{jk} and G'_k replacing G_k .

3. Implementation

Procedure MC decribes an algorithm that one can use to encode the essential steps for simulating k replications in parallel with initial state a and absorbing state b . In practice, one will want to embellish this procedure to allow for multiple reward functions and multiple independent macroreplications. The latter enable one to estimate variances and covariances of interest.

Figure 1 lists a FORTRAN subprogram called CHAIN that enables one to simulate an (N + 1) state Markov chain with state space on the integers 0,1,...,N using the parallel rotation sampling plan (7) for the purpose of computing sample mean rewards RPRIME(1),...,RPRIME(L) for L reward matrices stored in array A(·) . Each of I independent *macroreplications* begins with a departure of K correlated *microreplications* from state INITAL and ends with the absorption of all K microreplications in state ABSORB. The purpose of the macroreplications is to facilitate the estimation of the covariance matrix of the L sample mean reward functions. Also, CHAIN estimates the first passage time distribution from INITAL to ABSORB.

Insert Fig. 1 about here.

Procedure MC

Given: a, b, k, n, $\{s_i; i=0,\ldots,n\}$, $\{m_{ir}: r=1,\ldots,s_i; i=0,\ldots,n\}$,
$\{p_{i,m_{ir}}: r=1,\ldots,s_i; i=0,\ldots,n\}$ and $\{A_{im_{ir}}; r=1,\ldots,s_i, i=0,\ldots,n\}$.

1. $i \leftarrow a$.

2. $R' \leftarrow 0$.

3. $K'_a \leftarrow k$.

4. For $i=0,\ldots,n$

$\qquad$ For $r=1,\ldots,s_i$

$$q_{i,m_{ir}} \leftarrow \sum_{\ell=1}^{s_i} p_{i,m_{i\ell}}\;.$$

$$K^*_i \leftarrow 0\;.$$

$\left.\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array}\right\}$ Initialize.

5. Go to 8.

6. $i \leftarrow 0$.

7. If $i=b$ or $K'_i = 0$ go to 23.　　(Skip if state is absorbing or empty.)

8. $r \leftarrow 1$.

9. Sample U from $U(0,1)$.

10. $P^* \leftarrow 0$.

11. $\overline{P} \leftarrow 0$.

12. $Q \leftarrow K'_i\, q_{i,m_{ir}}$.

13. $Q^* \leftarrow \lfloor Q \rfloor$.

14. $\overline{Q} \leftarrow Q - Q^*$.

15. $X \leftarrow Q^* - P^* + \frac{1}{2}\,[\text{sign}\,(U-\overline{P}) + \text{sign}\,(\overline{Q}-U)]$.

$\left.\begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \end{array}\right\}$ Rotation Sampling

16. $K^*_{m_{ir}} \leftarrow K^*_{m_{ir}} + X$.　　　　(X microreplications move from i to m_{ir}.)

17. $R' \leftarrow R' + X\,A_{i,m_{ir}}$.　　　　(Compute reward.)

18. $P^* \leftarrow Q^*$.

19. $\overline{P} \leftarrow \overline{Q}$.

20. If $i=b$, $K_b' \leftarrow 0$.   (In case $a = b$.)

21. $r \leftarrow r + 1$.

22. If $r \leq s_i$ go to 12.

23. $i \leftarrow i + 1$.

24. If $i \leq n$ go to 7.

25. $i \leftarrow 0$.

26. If $i=b$ go to 33.

27. $r \leftarrow 1$.

28. If $m_{ir} = b$, $K_b' \leftarrow K_b' + K_b^*$ and go to 30.   (Arrange for absorptions.)

29. $K_{m_{ir}}' \leftarrow K_{m_{ir}}^*$. (Move to transient states.)

30. $K_{m_{ir}}^* \leftarrow 0$.

31. $r \leftarrow r + 1$.

32. If $r \leq s_i$ go to 28.   (Are all moves from i completed?)

33. $i \leftarrow i + 1$.

34. If $i \leq n$ go to 26.

35. If $K_b' < k$ go to 6.   (Are all absorbed?)

36. $R' \leftarrow R'/k$ and deliver R' .

Figure 2 contains a partitioned list of the input to CHAIN. Figure 2a displays all arrays and variables for which an initial numerical assignment is necessary at the time at which CHAIN is called. Figure 2b contains all interim working arrays and Fig. 2c lists all output arrays.

Insert Fig. 2 about here.

Note that the arrays A, M and P are one-dimensional in the subprogram whereas their counterparts $\{A_{ij}\}$, $\{m_{ij}\}$ and $\{p_{ij}\}$ are doubly subscripted in Section 1. This reduction leads to a considerable space saving, especially when $\{A_{ij}\}$ $\{m_{ij}\}$ and $\{p_{ij}\}$ are sparse and N is large. In terms of storage space, CHAIN requires $O(4(ALL(L+4) + 2L(L+3) + 4NP + SIZE + 8TT))$ bytes for the arrays listed in Fig. 2. Also, CHAIN has an upper bound on mean execution time of $O(ALL \times I \times L \times \ln K)$.

CHAIN uses the GGUBS random number generator in IMSL (1977) with SEED as the seed or initial random number and returns SIZE uniform deviates on each call of the generator. By choosing the blocking factor SIZE to be large one reduces the frequency of calling GGUBS, thus reducing CPU time. However, the space requirement for the uniform deviates is 4*SIZE bytes. On a computer with limited space, one may select a small SIZE to accomodate the space constraint. More generally, an alternative random number generator can be substituted by GGUBS with little effort.

The input OLD also calls for explanation. After running CHAIN for, say I1 independent macroreplications each of K correlated microreplications, a user may find that the accuracy of the sample mean rewards is too low for intended purposes. By setting OLD = I1 on a second run,

choosing a new I > OLD , using the original K and restoring XBAR(*)
and COV(*,*) in the *driver program*, one can merge the sample output
from the first OLD macroreplications with that from the subsequent
I - OLD new macroreplications to produce a summary tableau. When this is
done, the resulting sample first passage time distribution is based on
the last I - OLD macroreplications only.

Macroreplication versus Microreplication

As Section 1 shows, rotation sampling applied to K parallel micro-
replications produces a covariance matrix whose convergence rate has an
upper bound $O((\ln K)^2/K^2)$ on a single macroreplication. Since a method
is not yet available for estimating this covariance matrix from a single
macroreplication, CHAIN resorts to running I independent macroreplica-
tions for the purpose of estimating the covariance matrix of the L
sample reward functions. Therefore, the covariance matrix has a con-
vergence rate bounded by $O((\ln K)^2 /IK^2)$ and a run time of $O(I \ln K)$
for fixed ALL and L . Clearly one wants a K substantially larger than
I . In the example to be described next $K = 2^{17}$ and $I = 2^3$, but other
compromises are equally reasonable.

4. <u>An Example</u>

To illustrate how the CHAIN subprogram works in practice, consider
the Markov chain associated with the M/M/1 queueing problem with finite
capacity n . In particular, the *state* of the chain denotes the number

of customers in the system. In this queueing problem interarrival times are i.i.d. from the exponential distribution with rate λ, service times are i.i.d. from the exponential distribution with rate $\omega > \lambda$ and there is a single server. For the corresponding Markov chain these specifications imply

$$P_{01} = 1$$

$$P_{i,i-1} = \frac{\omega}{\lambda+\omega} \qquad i=1,\ldots,n$$

$$P_{i,i+1} = \frac{\lambda}{\lambda+\omega} \qquad i=1,\ldots,n-1$$

$$P_{n,n} = \frac{\lambda}{\lambda+\omega}$$

with all other transition probabilities being zero.

As objectives consider the estimation of

W_1 = mean number in system.

W_2 = probability of one customer in the system.

W_3 = probability of two customers in the system.

W_4 = first passage time probability mass function for the Markov chain from the empty and idle state back to that state.

W_5 = distribution function associated with W_4 .

Let $\{A_{ij}(\ell)\}$ denote reward matrix ℓ and $R_k'(\ell)$ denote sample mean reward function ℓ based on using $\{A_{ij}(\ell)\}$ in (5b). Then one estimates W_1, W_2 and W_3 by

$$\hat{W}_1 = R'_k(1)/R'_k(2)$$

$$\hat{W}_2 = R'_k(3)/R'_k(2)$$

$$\hat{W}_3 = R'_k(4)/R'_k(2)$$

where

$$A_{i,i+1}(1) = \frac{i+1}{\lambda+\omega} \qquad\qquad i=0,\ldots,n-1$$

$$A_{i,i-1}(1) = \frac{i-1}{\lambda+\omega} \qquad\qquad i=1,\ldots,n$$

$$A_{n,n}(1) = \frac{n}{\lambda+\omega}$$

$$A_{10}(2) = \frac{1}{\lambda}$$

$$A_{i,i+1}(2) = \frac{1}{\lambda+\omega} \qquad\qquad i=0,\ldots,n-1$$

$$A_{i,i-1}(2) = \frac{1}{\lambda+\omega} \qquad\qquad i=2,\ldots,n$$

$$A_{n,n}(2) = \frac{1}{\lambda+\omega}$$

$$A_{10}(3) = \frac{\omega}{\lambda+\omega}$$

$$A_{12}(3) = \frac{\lambda}{\lambda+\omega}$$

$$A_{21}(4) = \frac{\omega}{\lambda+\omega}$$

$$A_{23}(4) = \frac{\lambda}{\lambda+\omega} \quad .$$

For W_4 and W_5 we use the estimators in (10). These are computed automatically by CHAIN.

Figure 3 shows a driver program designed to initialize all relevant

parameters and call CHAIN for this problem. Here LAM and W

correspond to λ and ω

Insert Fig. 3 about here.

---

respectively. As input we set

$$LAM = 0.9$$
$$W = 1.0$$
$$N = 49$$
$$INITAL = 0$$
$$ABSORB = 0$$
$$I = 2^3 = 8$$
$$K = 2^{17} = 131072$$
$$L = 4$$
$$SEED = 1234567$$
$$SIZE = 40000$$
$$TT = 50 \ .$$

Figure 4 shows the output of CHAIN for this problem. The ratio

estimators W_1, W_2 and W_3 together with their biases and variances can

---

Insert Fig. 4 about here.

---

be computed by hand or by a subsequent subroutine that uses XBAR and COV as input together with the formulae

$$E(\frac{Y}{X} - \frac{EX}{EX}) \doteq \frac{EY}{EX} \ [\frac{var\ X}{E^2\ X} - \frac{cov(X,Y)}{EX \cdot EY}]$$

and

$$var(Y/X) \doteq \frac{E^2Y}{E^2X} \ [\frac{var\ X}{E^2\ X} - \frac{2\ cov(X,Y)}{EX \cdot EY} + \frac{var\ Y}{E^2\ Y}] \ .$$

We have chosen to do them by hand. They are

$$\hat{W}_1 = 8.7396 \qquad \hat{W}_2 = .0905 \qquad \hat{W}_3 = .0814$$
$$E(\hat{W}_1 - W_1) \doteq -.1037 \times 10^{-4} \quad E(\hat{W}_2 - W_2) \doteq .4304 \times 10^{-7} \quad E(\hat{W}_3 - W_3) \doteq .3735 \times 10^{-7}$$
$$var\ \hat{W}_1 \doteq .2646 \times 10^{-3} \quad var\ \hat{W}_2 \doteq .3780 \times 10^{-8} \quad var\ \hat{W}_3 \doteq .2936 \times 10^{-8} \ .$$

From Gross and Harris (1974, Sec. 2.5) one has

$$W_1 = 8.7410 \qquad W_2 = .0905 \qquad W_3 = .0814 \ ,$$

which confirm the performance of CHAIN.

All computing was performed on an IBM 370/155 computer. For FORTRAN G (level 21), the CHAIN Program requires 8592 bytes of space. For FORTRAN H (level 21.8) it requires 7380 bytes.

5. Restarting the Simulation

Situations will occur in which a user of CHAIN does not have a good
a priori estimate of the running time or the statistical reliability
to be expected from a specified set of I_1 macroreplications each of K_1
microreplications. At least two alternatives exist for dealing with this
case. A user may make a preliminary run and determine that I_2 additional
macroreplications, each of $K_2 = K_1$ microreplications, are necessary to
achieve the desired accuracy within budget. CHAIN is designed to accommodate
this alternative and, provided that the sample means and covariances accumu-
lated on the first I_1 macroreplications are restored prior to collecting the
additional I_2 macroreplications, the routine prints the global sample
means and covariances at the end of all $I_1 + I_2$ macroreplications.

The second alternative arises when on the basis of the first run a
user determines that I_2 macroreplications each of $K_2 \neq K_1$ microrepli-
cations is the most desirable way of achieving the desired accuracy. Here
the restoration feature of CHAIN does not apply. Let $\overline{X}$ and $\underset{\sim}{\Sigma}$ be the
sample mean vector and sample covariance matrix of $\underset{\sim}{\overline{X}}$ obtained on the
first run with I_1 and K_1. Let $\underset{\sim}{Y}$ and $\underset{\sim}{\Omega}$ denote the corresponding
quantities on the second run with I_2 and K_2. Then the overall sample
mean vector is

$$\underset{\sim}{\overline{Z}} = \frac{1}{(I_1 + I_2)} (I_1 \underset{\sim}{\overline{X}} + I_2 \underset{\sim}{\overline{Y}})$$

and its sample covariance matrix is

$$\underset{\sim}{\Gamma} = \frac{1}{(I_1 + I_2)^2} (I_1^2 \underset{\sim}{\Sigma} + I_2^2 \underset{\sim}{\Omega}) .$$

Although the computation of $\underset{\sim}{Z}$ and $\underset{\sim}{\Gamma}$ are not features of CHAIN one can easily add them if desired. However, as in the case of the ratio estimators in Section 4, the relative importance of this feature will differ from user to user.

References

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```
      SUBROUTINE CHAIN(K,OLD,I,NP,INITAL,ABSORB,S,B,SUMS,ALL,P,          00000100
     1              KPRIME,KSTAR,Q,L,ASIZE,A,RPRIME,XBAR,COV,COEFF,       00000110
     2              TT,FRBAR,FRVAR,CUMBAR,CUMVAR,SEED,SIZE,V)             00000120
C *** PROGRAM FOR SIMULATION OF MARKOV CHAIN WITH N+1 STATES             00000130
C *** USING ROTATION SAMPLING.                                           00000140
                                                                         00000150
      INTEGER NP,ABSORB,ALL,B,COUNT,I,INITAL,ISEED,IT,J,KPRIME(NP),      00000160
     1        KSTAR(NP),L,LA,LI,LIJ,K,LL,LH,R,M(ALL),N,OLD,OMEGA,X,      00000170
     2        PSTAR,QSTAR,OMEGA,SEED,SIZE,S(NP),SJ,SK,SS,SUMS(NP),TT,    00000180
     3        ASIZE                                                      00000190
      REAL*4  A(ASIZE),FRCV,CUMCV,V(SIZE)                                00000200
      REAL*8  C,CC,COEFF(L),COV(L,L),P(ALL),PP,PBAR,Q(ALL),QQ,QBAR,      00000210
     1        RPRIME(L),RSEED,XBAR(L),U,FREQ,CUM,FRVAR(TT),FRBAR(TT),    00000220
     2        CUMBAR(TT),CUMVAR(TT),FF,FFVAR,REG                         00000230
                                                                         00000240
C *** DESCRIPTION OF VARIABLES -                                         00000250
C ***                                                                    00000260
C *** A(*)      = REWARD MATRIX                                          00000270
C *** ABSORB    = ABSORBING STATE                                       00000280
C *** ALL       = SUM OF S(J) FOR ALL J                                  00000290
C *** ASIZE     = SIZE OF A ARRAY                                        00000300
C *** B         = TEST VARIABLE                                          00000310
C *** C         = ((L1-1)/LI)                                            00000320
C *** CC        = ((LI-OLD-1)/(LI-OLD))                                  00000330
C *** COEFF(*)  = COEFFICIENTS OF VARIATION                              00000340
C *** COUNT     = UNIFORM DEVIATE COUNTER                                00000350
C *** COV(*,*)  = COVARIANCE MATRIX                                      00000360
C *** CUM       = ACCUMULATION OF FREQ                                   00000370
C *** CUMBAR(*) = MEAN OF CUM                                            00000380
C *** CUMCV     = COEFFICIENT OF VARIATION FOR CUM                       00000390
C *** CUMVAR(*) = VARIANCE OF CUM                                        00000400
C *** FF        = SAMPLE MEAN FOR FIRST PASSAGE                          00000410
C *** FFVAR     = SAMPLE VARIANCE FOR FIRST PASSAGE                      00000420
C *** FRBAR(*)  = MEAN OF FREQ                                           00000430
C *** FRCV      = COEFFICIENT OF VARIATION FOR FREQ                      00000440
C *** FREQ      = NUMBER OF NEW TRANSITIONS INTO ABSORBING STATE         00000450
C *** FRVAR(*)  = VARIANCE OF FREQ                                       00000460
C *** I         = DESIRED NUMBER OF MACROREPLICATIONS                    00000470
C *** INITAL    = INITIAL STATE                                          00000480
C *** ISEED     = INITIAL SEED                                           00000490
C *** IT        = TRANSITION COUNTER                                     00000500
C *** J         = INDEX FOR STATES                                       00000510
C *** K         = NUMBER OF PARALLEL MICROREPLICATIONS                   00000520
C *** KPRIME(*) = NUMBER IN STATE AT END OF TRANSITION                   00000530
C *** KSTAR(*)  = NEXT KPRIME(*)                                         00000540
C *** L         = NUMBER OF DESCRIPTORS TO BE ESTIMATED                  00000550
C *** LA        = LL + 1                                                 00000560
C *** LI        = INDEX FOR I                                            00000570
C *** LIJ       = 1 + OLD                                                00000580
C *** LJ        = INDEX FOR STATES                                       00000590
```

Fig. 1. CHAIN Subroutine

```
C *** LL        = INDEX FOR L                                      00000600
C *** LB        = INDEX FOR L                                      00000610
C *** R(*)      = STATES THAT CAN BE ENTERED FROM J-1              00000620
C *** N         = NUMBER OF HIGHEST STATE                          00000630
C *** NI        = NUMBER OF STATES (N+1)                           00000640
C *** OLD       = NUMBER OF MACROREPLICATIONS ALREADY PERFORMED (OLD<I) 00000650
C *** OMEGA     = TEST VARIABLE                                    00000660
C *** P(*)      = TRANSITION MATRIX                                00000670
C *** PP        = QQ FROM TIME BEFORE                              00000680
C *** PBAR      = FRACTIONAL PART OF PP                            00000690
C *** PSTAR     = INTEGER PART OF PP                               00000700
C *** Q(*)      = FROM P                                           00000710
C *** QQ        = FROM Q AND K                                     00000720
C *** QBAR      = FRACTIONAL PART OF QQ                            00000730
C *** QSTAR     = INTEGER PART OF QQ                               00000740
C *** R         = INDEX FOR STATES                                 00000750
C *** REG       = ACCUMULATED FREQ FOR TRANSITIONS GREATER THAN TT-1 00000760
C *** RPRIME(*) = CUMULATIVE REWARD FOR ESTIMATORS                 00000770
C *** RSEED     = RANDOM GENERATOR SEED, REAL VALUED               00000780
C *** SEED      = RANDOM GENERATOR SEED                            00000790
C *** SIZE      = BLOCK SIZE FOR RANDOM NUMBER GENERATOR           00000800
C *** S(J)      = NUMBER OF STATES THAT CAN BE ENTERED FROM J-1    00000810
C *** SJ        = S(J)                                             00000820
C *** SK        = SUMS(J)                                          00000830
C *** SS        = MIN (NUMBER OF TRANSITIONS, TT)                  00000840
C *** SUMS(J)   = SUM OF S(1) THRU S(J-1), AND SUMS(1)=0           00000850
C *** TT        = MAXIMUM NUMBER OF TRANSITIONS TO LOOK AT         00000860
C *** U         = CURRENT UNIFORM DEVIATE                          00000870
C *** V(*)      = UNIFORM DEVIATE ARRAY                            00000880
C *** X         = NUMBER OF TRANSITIONS IN CURRENT MOVE            00000890
C *** XBAR(*)   = MEAN MATRIX                                      00000900
C                                                                  00000910
C *** INITIALIZE VARIABLES.                                        00000920
C                                                                  00000930
      PP    = 0.0D0                                                00000940
      PPVAR = 0.0D0                                                00000950
      SS    = 0                                                    00000960
      ISEED = SEED                                                 00000970
      RSEED = SEED                                                 00000980
      COUNT = SIZE                                                 00000990
      DO 80 J=1,TT                                                 00001000
         PPVAR(J)   = 0.0D0                                        00001010
         PPBAR(J)   = 0.0D0                                        00001020
         CUMVAR(J)  = 0.0D0                                        00001030
80       CUMBAR(J)  = 0.0D0                                        00001040
      DO 100 J=1,NP                                                00001050
         SK          = SUMS(J)                                     00001060
         Q(SK+1)     = P(SK+1)                                     00001070
         IF (S(J).LT.2) GO TO 100                                  00001080
         SJ          = S(J)                                        00001090
```

Fig. 1 *(Continued)*

```
           DO   90 R=2,SJ                                              00001100
  90          Q(SK+R) = Q(SK+R-1)+P(SK+R)                              00001110
              Q(SK+SJ)   = 1.0000D0                                    00001120
 100          CONTINUE                                                 00001130
C *** CHECK IF XBAR AND COV ARE RESTORED.                             00001140
       IF (OLD.GT.0) GO TO 115                                         00001150
       DO 110 LL=1,L                                                   00001160
          XBAR(LL)    = 0.0D0                                          00001170
          COEFF(LL)   = 0.0D0                                          00001180
          DO 110 LM=1,L                                                00001190
 110         COV(LL,LM) = 0.0D0                                        00001200
 115   LIJ = 1 + OLD                                                   00001210
       DO 118 LL=1,L                                                   00001220
          XBAR(LL) = XBAR(LL)*OLD                                      00001230
          DO 118 LM=1,L                                                00001240
 118         COV(LL,LM) = COV(LL,LM)*OLD                               00001250
                                                                       00001260
C *** START MAIN LOOP.                                                00001270
       DO 540 LI=LIJ,I                                                 00001280
C *** INITIALIZE VARIABLES FOR THIS REPLICATION.                      00001290
          B       = 0                                                  00001300
          C       = (LI-1.0D0)/LI                                      00001310
          CC      = (LI-OLD-1.0D0)/(LI-OLD)                            00001320
          CUM     = 0.0D0                                              00001330
          REG     = 0.0D0                                              00001340
          IT      = 1                                                  00001350
          OMEGA = 0                                                    00001360
          DO 120 LL=1,L                                                00001370
 120         RPRIME(LL) = 0.0D0                                        00001380
          DO 130 J=1,NP                                                00001390
             KSTAR(J) = 0                                              00001400
 130         KPRIME(J) = 0                                             00001410
C *** START THIS REPLICATION WITH ALL MICROREPLICATIONS IN INITIAL STATE00001420
          J       = INITAL + 1                                         00001430
          KPRIME(J)= K                                                 00001440
          KSTAR(J) = K                                                 00001450
C *** LOOK AT INITIAL STATE.                                          00001460
          J       = INITAL + 1                                         00001470
          GO TO 400                                                    00001480
C *** LOOK AT THE NEXT STATE.                                         00001490
 300      J       = J+1                                                00001500
C *** SKIP THE ABSORBING STATE.                                      00001510
          IF (J.EQ.ABSORB+1) J = J+1                                  00001520
C *** IF NONE IN THIS STATE, LOOK AT THE NEXT STATE.                 00001530
 400      IF (KPRIME(J).EQ.0) GO TO 300                               00001540
C *** FIND THE NUMBER OF STATES THAT CAN BE ENTERED FROM STATE J-1.  00001550
          SJ      = S(J)                                               00001560
C *** START WITH THE FIRST STATE THAT CAN BE ENTERED FROM STATE J-1. 00001570
          K       = 1                                                  00001580
C *** POINT TO THE NEXT DEVIATE TO USE.                              00001590
```

Fig. 1 (*Continued*)

```
        COUNT = COUNT + 1                                              00001600
C *** GET NEW ARRAY OF DEVIATES IF NEEDED.                             00001610
        IF (COUNT.LE.SIZE) GO TO 420                                   00001620
        COUNT = 1                                                      00001630
C ***   CALL RANDOM(SEED,V,SIZE)                                       00001640
        CALL GGUBS(RSEED,SIZE,V)                                       00001650
C *** GET THE DEVIATE POINTED TO BY COUNT.                             00001660
C *** TRANSFORM DEVIATE.                                               00001670
420     U        = DBLE(AMOD(KPRIME(J)*V(COUNT),1.))                   00001680
C       WRITE(3,2040) U,V(COUNT)                                       00001690
C *** TRANSFER ALL OUT OF THIS STATE FOR TRANSITIONS.                  00001700
        KSTAR(J) = KSTAR(J) - KPRIME(J)                                00001710
C *** INITIALIZE QQ, QSTAR, AND QBAR.                                  00001720
        QQ    = 0.0                                                    00001730
        QSTAR = 0                                                      00001740
        QBAR  = 0.0                                                    00001750
C *** SAVE THE LAST OCCURRENCE OF QQ, QSTAR, AND QBAR.                 00001760
500     PP    = QQ                                                     00001770
        PSTAR = QSTAR                                                  00001780
        PBAR  = QBAR                                                   00001790
C *** COMPUTE NEW VALUES FOR QQ, QSTAR, AND QBAR.                      00001800
        QQ    = KPRIME(J)*U(SUMS(J)+R)                                 00001810
        QSTAR = IDINT(QQ)                                              00001820
        QBAR  = DMOD(QQ,1.0D0)                                         00001830
C *** FIND THE # OF TRANSITIONS TO THE R-TH STATE THAT CAN BE ENTERED. 00001840
C *** FROM J-1.                                                        00001850
        X        = (QSTAR-PSTAR)+.5*(DSIGN(1.0D0,U-PBAR)+              00001860
     1                              DSIGN(1.0D0,QBAR-U))               00001870
C *** ADD THESE TRANSITIONS TO THE ENTERED STATE OCCUPANCY VECTOR.     00001880
        KSTAR(M(SUMS(J)+R)+1) = KSTAR(M(SUMS(J)+R)+1)+X                00001890
C *** FIND THE NUMBER OF TRANSITIONS MADE SO FAR FOR THIS STATE.       00001900
        B        = B+X                                                 00001910
C *** ACCUMULATE THE REWARDS FOR THIS STATE TRANSITION.                00001920
        DO 510 LL=1,L                                                  00001930
          IF (A(ALL*(LL-1)+SUMS(J)+R).EQ.0.0.OR.X.EQ.0) GO TO 510     00001940
          RPRIME(LL) = RPRIME(LL)+A(ALL*(LL-1)+SUMS(J)+R)*X           00001950
510       CONTINUE                                                    00001960
C *** GO TO THE NEXT STATE THAT CAN BE REACHED FROM J-1.               00001970
        R     = R+1                                                    00001980
C *** IF NOT ALL TRANSITIONS WERE MADE FOR THIS STATE, TRY AGAIN.      00001990
        IF (B.LT.KPRIME(J)) GO TO 500                                 00002000
C *** ACCUMULATE THE NUMBER OF TRANSITIONS MADE SO FAR FOR ALL STATES. 00002010
        OMEGA = OMEGA+B                                                00002020
C *** CLEAR THE NUMBER OF TRANSITIONS FOR THE STATE COUNTER.           00002030
        B     = 0                                                      00002040
C *** IF NOT ALL TRANSITIONS WERE MADE YET, TRY AGAIN.                 00002050
        IF (OMEGA.LT.K-KPRIME(ABSORB+1)) GO TO 300                    00002060
        OMEGA = 0                                                      00002070
C *** ACCUMULATE FBBAR, FBVAR, CUMBAR AND CUMVAR.                      00002080
        FREQ = KSTAR(ABSORB+1)-KPRIME(ABSORB+1)                       00002090
```

Fig. 1 *(Continued)*

```
          IF (IT.EQ.1) FREQ = KSTAR(ABSORB+1)                   00002100
          FF        = FF + IT*FREQ                              00002110
          FFVAR     = FFVAR + IT**2*FREQ                        00002120
          CUM  = CUM + FREQ                                     00002130
          LL   = MINO(TT,IT)                                    00002140
          IF (IT.LT.TT) GO TO 515                               00002150
          REG  = REG + FREQ                                     00002160
          IF (KSTAR(ABSORB+1).LT.K) GO TO 522                   00002170
          FREQ = REG                                            00002180
515       FRBAR(LL)  = FRBAR(LL) + FREQ                         00002190
          CUMBAR(LL) = CUMBAR(LL) + CUM                         00002200
          FRVAR(LL)  = FRVAR(LL) + FREQ**2                      00002210
          CUMVAR(LL) = CUMVAR(LL) + CUM**2                      00002220
C *** RESET THE STATE OCCUPANCY VECTOR.                         00002230
522       DO 525 LJ=1,NP                                        00002240
          KPRIME(LJ) = KSTAR(LJ)                                00002250
          SJ     = S(LJ)                                        00002260
          DO 525 B=1,SJ                                         00002270
525       KPRIME(M(SUBS(LJ)+B)+1) = KSTAR(M(SUBS(LJ)+B)+1)      00002280
C *** START NEXT TRANSITION IN STATE 0.                         00002290
          J = 0                                                 00002300
C *** COMPUTE THE NUMBER OF TRANSITIONS MADE SO FAR.            00002310
          IT = IT + 1                                           00002320
C *** IF NOT ALL ABSORBED, TRY AGAIN.                           00002330
          IF (KPRIME(ABSORB+1).LT.K) GO TO 300                  00002340
C *** RECURSIVE COMPUTATIONS.                                   00002350
          IF (LL.GE.TT) GO TO 529                                00002360
C *** ACCUMULATE CUMBAR AND CUMVAR FOR # OF TRANSITION STEPS > TT-1. 00002370
          LL = LL + 1                                           00002380
          DO 527 LM=LL,TT                                       00002390
          CUMVAR(LM) = CUMVAR(LM) + CUM**2                      00002400
527       CUMBAR(LM) = CUMBAR(LM) + CUM                         00002410
C *** COMPUTE THE COVARIANCE MATRIX RECURSIVELY.                00002420
529       IF (LI.EQ.1) GO TO 535                                00002430
          DO 530 LL=1,L                                         00002440
          DO 530 LM=1,L                                         00002450
530       COV(LL,LM)=((LI-2)*COV(LL,LM)+(RPRIME(LL)/K-XBAR(LL))* 00002460
     1              (RPRIME(LM)/K-XBAR(LM))*C)/(LI-1)           00002470
C *** COMPUTE SS.                                               00002480
535       SS = MINO(TT,MAXO(SS,IT-1))                           00002490
C *** COMPUTE THE SAMPLE MEAN VECTOR RECURSIVELY.               00002500
          DO 540 LL=1,L                                         00002510
          XBAR(LL) = C*XBAR(LL)+(1.0D0-C)*RPRIME(LL)/K          00002520
540       CONTINUE                                              00002530
                                                                00002540
C *** END MAIN LOOP, COMPLETED I MACROREPLICATIONS.             00002550
C ***                                                           00002560
C *** COMPUTE FRBAR, FRVAR, CUMBAR, AND CUMVAR DIRECTLY.        00002570
          IF (I.NE.1) REG = (K**2.0D0)*(I**2.0D0)*(I-1.0D0)     00002580
          DO 545 LL=1,TT                                        00002590
```

Fig. 1 (*Continued*)

```
          IF (I.EQ.1) GO TO 544                                          00002600
          PRVAR(LL)   = (I*PRVAR(LL)-PRBAR(LL)**2)/REG                   00002610
          CUMVAR(LL)  = (I*CUMVAR(LL)-CUMBAR(LL)**2)/REG                 00002620
544       CUMBAR(LL)  = CUMBAR(LL)/(K*I)                                 00002630
545       PRBAR(LL)   = PRBAR(LL)/(K*I)                                  00002640
                                                                         00002650
      DO 550 LL=1,L                                                      00002660
          DO 550 LM=1,L                                                  00002670
550          COV(LL,LM) = COV(LL,LM)/L                                   00002680
      DO 570 LL=1,L                                                      00002690
          IF (XBAR(LL).NE.0) COEFF(LL) = DSQRT(COV(LL,LL))/XBAR(LL)      00002700
          IF (LL.EQ.L) GO TO 570                                         00002710
          LA = LL+1                                                      00002720
          DO 560 LM=LA,L                                                 00002730
             IF (COV(LL,LL)*COV(LM,LM).GT.0)                             00002740
     1          COV(LM,LL)=COV(LL,LM)/DSQRT(COV(LL,LL)*COV(LM,LM))       00002750
560          CONTINUE                                                    00002760
570       CONTINUE                                                       00002770
                                                                         00002780
C *** PRINT RESULTS.                                                     00002790
                                                                         00002800
      SEED = MSEED                                                       00002810
      WRITE (3,1000) NP,INITAL,ABSORB,ALL,L,K,I,ISEED,SEED,SIZE          00002820
1000  FORMAT(1H1,'RESULTS OF ROTATION SAMPLING FOR A MARKOV CHAIN',///,  00002830
     1' NO. OF STATES                       =',I10//,                    00002840
     2' INITIAL STATE                       =',I10//,                    00002850
     3' ABSORBING STATE                     =',I10//,                    00002860
     4' TOTAL NO. OF (I,J) PAIRS            =',I10//,                     00002870
     5' NO. OF DESCRIPTORS                  =',I10//,                     00002880
     6' NO. OF CORRELATED MICROREPLICATIONS =',I10//,                    00002890
     7' NO. OF INDEPENDENT MACROREPLICATIONS =',I10//,                   00002900
     8' INITIAL SEED                        =',I10//,                    00002910
     9' FINAL SEED                          =',I10//,                    00002920
     C' BLOCKING FACTOR                     =',I10/)                     00002930
      REWIND 11                                                          00002940
      WRITE (3,2000)                                                     00002950
      WRITE (3,2030)                                                     00002960
      WRITE (3,2040) (XBAR(LL),LL=1,L)                                   00002970
      WRITE (3,2010)                                                     00002980
      WRITE (3,2030)                                                     00002990
      WRITE (3,2040) (COEFF(LL),LL=1,L)                                  00003000
      WRITE (3,2020)                                                     00003010
      WRITE (3,2030)                                                     00003020
      DO 580 LL=1,L                                                      00003030
          WRITE (3,2045) LL, (COV(LL,LM),LM=1,L)                         00003040
580   CONTINUE                                                           00003050
2000  FORMAT(//,' SAMPLE MEAN VECTOR',/,                                 00003060
     1        ' ******************',/)                                   00003070
2010  FORMAT(//,' SAMPLE COEFFICIENTS OF VARIATION',/,                   00003080
     1        ' ********************************',/)                     00003090
```

Fig. 1 (*Continued*)

```
2020   FORMAT(//,' SAMPLE COVARIANCE/CORRELATION MATRIX',/,      00003100
   1        ' **** *** ********************************',/)        00003110
2030   FORMAT(9X,'1',14X,'2',14X,'3',14X,'4',14X,'5',14X,'6',14X,'7',  00003120
   1        14X,'8',14X,'9',//)                                   00003130
2040   FORMAT(2X,9(D15.8)/)                                       00003140
2045   FORMAT(I2,9(D15.8)/)                                       00003150
       FF       = FF/(K*I)                                        00003160
       FFVAR    = FFVAR/(K*I) - FF**2                             00003170
       DO 620 LL=1,SS                                             00003180
          FRCV = 0.0                                              00003190
          CUMCV = 0.0                                             00003200
          IF (FRBAR(LL).NE.0.0D0) FRCV=DSQRT(FRVAR(LL))/FRBAR(LL)  00003210
          IF (CUMBAR(LL).NE.0.0D0) CUMCV=DSQRT(CUMVAR(LL))/CUMBAR(LL) 00003220
          IF (MOD(LL,50).NE.1) GO TO 620                          00003230
          WRITE (3,3000)                                          00003240
          IF (LL.GT.1) GO TO 610                                  00003250
          WRITE (3,3010) FF,FFVAR                                 00003260
610       WRITE (3,3020)                                          00003270
620       WRITE (3,3030) LL,FRBAR(LL),FRVAR(LL),FRCV,CUMBAR(LL),  00003280
   1                     CUMVAR(LL),CUMCV                         00003290
       IF (OLD.EQ.0) RETURN                                       00003300
       LL = I - OLD                                               00003310
       WRITE (3,4000) LL                                          00003320
3000   FORMAT(1H1,'FIRST PASSAGE TIME (T) DISTRIBUTION',/,        00003330
   1        ' ******************************************')        00003340
3010   FORMAT(/,1X,'SAMPLE MEAN(T) =',D15.8,5X,                   00003350
   1        'SAMPLE VARIANCE(T) =',D15.8)                         00003360
3020   FORMAT(/,33X,'MASS FUNCTION',42X,'DISTRIBUTION FUNCTION',//,  00003370
   1                          35X,'VARIANCE',10X,'COEFFICIENT',   00003380
   2                          31X,'VARIANCE',10X,'COEFFICIENT',/,  00003390
   3     '   I',10X,'PR(T=I)',11X,'OF PR(T=I) ',9X,'OF VARIATION',  00003400
   4           10X,'PR(T<=I)',10X,'OF PR(T<=I)',9X,'OF VARIATION',  00003410
   5     /,'   ---',9X,'-------',11X,'-------------',9X,'------------',  00003420
   6           10X,'--------',10X,'-----------',9X,'------------')  00003430
3030   FORMAT(' ',I5,6(5X,D15.8))                                 00003440
4000   FORMAT(/,' FIRST PASSAGE DISTRIBUTION IS BASED ON THE LAST ',  00003450
   1        I5,' MACROREPLICATIONS.')                             00003460
       RETURN                                                     00003470
       END                                                        00003480
```

Fig. 1 *(Continued)*

Fig. 2   Input to CHAIN Subprogram

(a) Data Input

VARIABLE	TYPE	DESCRIPTION
A	REAL*4(ASIZE)	A(ALL*(LL-1) + SUMS(J) + R) = reward received when a replication jumps from state J - 1 to state M(SUMS(J) + R) for R = 1,...,S(J) for reward function LL = 1,2,...,L
ABSORB	INTEGER	Absorbing state 0 ≤ ABSORB ≤ N + 1
ALL	INTEGER	Total number of arcs = SUMS(NP) + S(NP)
ASIZE	INTEGER	ALL*L
I	INTEGER	Desired number of independent macroreplications
INITAL	INTEGER	Initial state 0 ≤ INITAL ≤ N + 1
K	INTEGER	Number of parallel microreplications per macroreplication
L	INTEGER	Total number of reward functions
M	INTEGER(N+1)	M(SUM(J) + LR) = LRth of S(J) states to which a replication can move from state J - 1 LR = 1,...,S(J)
NP	INTEGER	NP = N + 1 = total number of states
OLD	INTEGER	If OLD = 0 simulation proceeds to run I macro-replications If OLD > 0 simulation proceeds to run I - OLD additional macroreplications
P	REAL*4(ALL)	P(SUM(J) + LR) = probability of moving from state J - 1 to M(SUM(J) + LR) LR = 1,...,S(J)
S	INTEGER(N+1)	S(J) = number of states that can be entered from state J - 1
SEED	INTEGER	Initial value for random number generator
SIZE	INTEGER	Each call to the random number generator returns a block of SIZE uniform deviates

Fig. 2 *(Continued)*

(a)

VARIABLE	TYPE	DESCRIPTION
SUMS	INTEGER(NP)	$SUMS(J) = 0 \qquad J = 1$ $\qquad = \sum_{I=1}^{J-1} S(I) \qquad J = 2,\ldots,NP$
TT	INTEGER	Number of cells in sample first passage time distribution. Last cell estimates probability of absorption at time $\geq$ TT

(b) Working Arrays

VARIABLE	TYPE	DESCRIPTION
KPRIME	INTEGER(NP)	Distribution of microreplications by state at end of a transition
KSTAR	INTEGER(NP)	Distribution of microreplications by state at beginning of a transition
Q	REAL*8(ALL)	Q(SUM(J) + LR) = probability of moving from state $J - 1$ to state M(SUM(J) + 1), M(SUM(J) + 2),... or M(SUM(J) + LR) LR = 1,...,S(J)
RPRIME	REAL*8(L)	Accumulated rewards for L reward functions
V	REAL*4(SIZE)	Space to store uniform deviates

Fig. 2 (*Continued*)

(c) Arrays Used to Summarize Data on I Macroreplications

VARIABLE	TYPE	DESCRIPTION
COEFF	REAL*8(L)	COEFF(J1) = sample coefficient of variation of XBAR(J1) J1=1,...,L
COV	REAL*8(L,L)	At completion COV(J1, J2) contains the sample covariance of XBAR(J1) and XBAR(J2) for J2=J1,...,L and J1=1,...,L and COV(J2,J1) contains the sample correlation between XBAR(J1) and XBAR(J2) for J1=1,...,J2-1 and J2=2,...,L .
CUMBAR	REAL*8(TT)	CUMBAR(J1) = sample probability that absorption occurs on a step ≤ J1 for J1=1,...,TT - 1; CUMBAR(TT) = 1
CUMVAR	REAL*8(TT)	CUMVAR(J1) = Sample variance of CUMBAR(J1) J1=1,...,TT
FF	REAL*8	Sample mean of first passage time.
FFVAR	REAL*8	Sample variance of first passage time.
FRBAR	REAL*8(TT)	FRBAR(J1) = sample absorption probability at step J1 for J1=1,...,TT - 1 $$FRBAR(TT) = 1 - \sum_{J1=1}^{TT-1} FRBAR(J1)$$
FRVAR	REAL*8(TT)	FRVAR(J1) = sample variance of FRBAR(J1) J1=1,...,TT
XBAR	REAL*8(L)	XBAR(J1) = the sample mean reward for reward function J1=1,...,L

```
      INTEGER I,J,KPRIME(50),KSTAR(50),L,K,LL,M(100),N,NP,S(50),      00000100
     1       SUMS(50),ALL,INITAL,ABSORB,SIZE,OLD,SEED,TT,ASIZE          00000110
      REAL*4  A(500),LAM,V(40000),W                                     00000120
      REAL*8  COEPP(10),COV(10,10),Q(100),PRIME(10),XBAR(10),           00000130
     1        P(100),PRVAR(100),PRBAR(100),CUMBAR(100),CUMVAR(100)      00000140
                                                                        00000150
C *** INITIALIZE VALUES.                                                00000160
                                                                        00000170
      READ (1,1000) N,L,K,LAM,W,I,ABSORB,INITAL,SIZE,TT                 00000180
1000  FORMAT (I5,/,I3,/,I6,/,F4.1,/,F4.1,/,I5,/,I5,/,I5,/,I5,/,I5)      00000190
      WRITE(3,1005) N,L,K,LAM,W,I,ABSORB,INITAL,SIZE,TT                 00000200
1005  FORMAT (' N=',I5,' L=',I3,' K=',I6,                              00000210
     1        ' LAM=',F4.1,' W=',F4.1,' I=',I5,' ABSORB=',I5,          00000220
     2        ' INITAL=',I5,' SIZE=',I5,' TT=',I5)                     00000230
      NP = N + 1                                                        00000240
      READ (11,1020) SEED                                               00000250
1020  FORMAT(I10)                                                       00000260
C *** FOR EACH STATE DETERMINE THE NUMBER OF STATES THAT CAN BE ENTERED.00000270
      S(1) = 1                                                          00000280
      DO 80 J=2,NP                                                      00000290
80        S(J) = 2                                                      00000300
      WRITE(3,1015) (S(J),J=1,NP)                                       00000310
1015  FORMAT (' S(J)      =',20I5)                                      00000320
      SUMS(1) = 0                                                       00000330
      ALL     = S(1)                                                    00000340
      DO 90 J=2,NP                                                      00000350
         SUMS(J) = ALL                                                  00000360
90       ALL     = ALL + S(J)                                          00000370
C *** THE NEXT INITIALIZATIONS MAY BE RUN SPECIFIC.                     00000380
      OLD = 0                                                           00000390
      DO 100 J=2,NP                                                     00000400
C ***    COMPUTE TRANSITION PROBABILITIES.                             00000410
         P(SUMS(J)+1) =   W/(LAM+W)                                    00000420
         P(SUMS(J)+2) = LAM/(LAM+W)                                    00000430
100      CONTINUE                                                      00000440
      P(1)          = 1.0                                              00000450
      WRITE (3,1016) (P(LW),LW=1,ALL)                                  00000460
1016  FORMAT (' P(*)     =',20F5.2)                                    00000470
C *** FOR EACH STATE J DETERMINE STATES THAT CAN BE ENTERED.           00000480
      DO 400 J=2,N                                                     00000490
         M(SUMS(J)+1) = J-2                                            00000500
400      M(SUMS(J)+2) = J                                              00000510
      M(1)          = 1                                                00000520
      M(SUMS(NP)+1) = N-1                                              00000530
      M(SUMS(NP)+2) = N                                                00000540
      WRITE (3,1017) (M(LL),LL=1,ALL)                                  00000550
1017  FORMAT (' M(*)     =',20I5)                                      00000560
C *** COMPUTE REWARD VECTOR.                                           00000570
      DO 500 J=1,NP                                                    00000580
         A(ALL*2+SUMS(J)+1) = 0.0                                      00000590
```

Fig. 3 Driver Routine for Example

```
       A(ALL*2+SUMS(J)+2)  = 0.0                                    00000600
       A(ALL*3+SUMS(J)+1)  = 0.0                                    00000610
       A(ALL*3+SUMS(J)+2)  = 0.0                                    00000620
       A(SUMS(J)+1)        = M(SUMS(J)+1)/(LAM+W)                   00000630
       A(SUMS(J)+2)        = M(SUMS(J)+2)/(LAM+W)                   00000640
       A(ALL+SUMS(J)+1)    = 1/(LAM+W)                              00000650
  500  A(ALL+SUMS(J)+2)    = 1/(LAM+W)                              00000660
     A(ALL+SUMS(2)+1)      = 1/LAM                                  00000670
     A(ALL*2+1)            = 1/(LAM+W)                              00000680
     A(ALL*2+SUMS(3)+1)    = 1/(LAM+W)                              00000690
     A(ALL*3+SUMS(2)+2)    = 1/(LAM+W)                              00000700
     A(ALL*3+SUMS(4)+1)    = 1/(LAM+W)                              00000710
       DO 550 LL=1,L                                                00000720
       WRITE (3,1018) (A(ALL*(LL-1)+LB),LB=1,ALL)                   00000730
 1018  FORMAT (' A(*,LL)   =',20F5.2)                               00000740
  550  CONTINUE                                                     00000750
       ASIZE = ALL*L                                                00000760
C ***  CALL PARALLEL SIMULATION PROGRAM.                            00000770
       CALL CHAIN(K,OLD,I,NP,INITAL,ABSORB,S,M,SUMS,ALL,P,KPRIME,   00000780
      1           KSTAR,U,L,ASIZE,A,PRIME,XBAR,COV,COEFF,TT,PRBAR,  00000790
      2           PRVAR,CUMBAR,CUMVAR,SEED,SIZE,V)                  00000800
       STOP                                                         00000810
       END                                                          00000820
```

Fig. 3 (*Continued*)

Fig. 4   Sample Output from CHAIN Subroutine

RESULTS OF ROTATION SAMPLING FOR A MARKOV CHAIN

NO. OF STATES	= 50
INITIAL STATE	= 0
ABSORBING STATE	= 0
TOTAL NO. OF (I,J) PAIRS	= 99
NO. OF DESCRIPTORS	= 4
NO. OF CORRELATED MICROREPLICATIONS	= 131072
NO. OF INDEPENDENT MACROREPLICATIONS	= 8
INITIAL SEED	= 1234567
FINAL SEED	= 590573803
BLOCKING FACTOR	= 40000

SAMPLE MEAN VECTOR
●●●●●●●●●●●●●●●●●●

1   2   3   4   5   6   7   8   9

0.96593610D 02 0.11052800D 02 0.99996355D 00 0.89989158D 00

SAMPLE COEFFICIENTS OF VARIATION
●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●

1   2   3   4   5   6   7   8   9

0.25163951D-02 0.70228364D-03 0.59198037D-04 0.13659310D-03

SAMPLE COVARIANCE/CORRELATION MATRIX
●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●●

1   2   3   4   5   6   7   8   9

1 0.59081904D-01 0.17939022D-02 0.37090189D-05 0.57659548D-05
2 0.95082860D 00 0.60247435D-04 0.19277545D-06 0.36303695D-06
3 0.25777124D 00 0.41955133D 00 0.35082468D-08 0.70713160D-08
8 0.19295446D 00 0.35954452D 00 0.97181561D 00 0.15109075D-07

Fig. 4 (Continued)

FIRST PASSAGE TIME (T) DISTRIBUTION

SAMPLE MEAN(T) = 0.19886985D 02   SAMPLE VARIANCE(T) = 0.64011433D 04

I	MASS FUNCTION			DISTRIBUTION FUNCTION		
	PR(T=I)	VARIANCE OF PR(T=I)	COEFFICIENT OF VARIATION	PR(T≤I)	VARIANCE OF PR(T≤I)	COEFFICIENT OF VARIATION
1	0.0	0.0	0.0	0.0	0.0	0.0
2	0.52631664D 00	0.19489172D-11	0.26524640E-05	0.52631664D 00	0.19489172D-11	0.26524640E-05
3	0.13121223D 00	0.15591138D-11	0.95162832E-05	0.52631664D 00	0.19489172D-11	0.26524640E-05
4	0.0	0.0	0.0	0.65752888D 00	0.40277623D-11	0.30522287E-05
5	0.65426026D-01	0.19489172D-11	0.21337357E-04	0.65752888D 00	0.40277623D-11	0.30522287E-05
6	0.0	0.0	0.0	0.72295570D 00	0.15591138D-11	0.17271495E-05
7	0.60778160D-01	0.29883397D-11	0.42392334E-04	0.72295570D 00	0.15591138D-11	0.17271495E-05
8	0.0	0.0	0.0	0.76373186D 00	0.50671048D-11	0.29474149E-05
9	0.28466225D-01	0.50671048D-11	0.79077596E-04	0.76373186D 00	0.50671048D-11	0.29474149E-05
10	0.0	0.0	0.0	0.79220009D 00	0.36379788D-11	0.24076598E-05
11	0.21200779D-01	0.19489172D-11	0.65569984E-04	0.81349087D 00	0.36379788D-11	0.24076598E-05
12	0.0	0.0	0.0	0.81349087D 00	0.29883397D-11	0.21250162E-05
13	0.16678010D-01	0.29883397D-11	0.10344536E-03	0.83016968D 00	0.29883397D-11	0.21250162E-05
14	0.0	0.0	0.0	0.83016968D 00	0.62365351D-11	0.30081865E-05
15	0.13518113D-01	0.29883397D-11	0.12787682E-03	0.84368001D 00	0.62365351D-11	0.30081865E-05
16	0.0	0.0	0.0	0.84368001D 00	0.29883397D-11	0.20499579E-05
17	0.11230469D-01	0.20788450D-11	0.12838467E-03	0.85491848D 00	0.29883397D-11	0.20499579E-05
18	0.0	0.0	0.0	0.85491848D 00	0.50671048D-11	0.26330472E-05
19	0.95224380D-02	0.90949470D-12	0.10015022E-03	0.86440920D 00	0.50671048D-11	0.26330472E-05
20	0.0	0.0	0.0	0.86440920D 00	0.83153801D-11	0.31358438E-05
21	0.81996918D-02	0.15591138D-11	0.15228045E-03	0.87264092D 00	0.83153801D-11	0.31358438E-05
22	0.0	0.0	0.0	0.87264061D 00	0.77956689D-11	0.31995669E-05
23	0.71525574D-02	0.20788450D-11	0.20158105E-03	0.87979317D 00	0.77956689D-11	0.31995669E-05
24	0.0	0.0	0.0	0.87979317D 00	0.77956689D-11	0.31735553E-05
25	0.63123703D-02	0.40277623D-11	0.31793560E-03	0.86105554D 00	0.77956689D-11	0.31735553E-05
26	0.0	0.0	0.0	0.86105554D 00	0.18579677D-10	0.48644779E-05
27	0.56290027D-02	0.19489172D-11	0.24840469E-03	0.89172554D 00	0.18579677D-10	0.48644779E-05
28	0.0	0.0	0.0	0.89172554D 00	0.18189894D-10	0.47828180E-05
29	0.50439835D-02	0.90949470D-12	0.18907165E-03	0.89676952D 00	0.18189894D-10	0.47828180E-05
30	0.0	0.0	0.0	0.89676952D 00	0.16500832D-10	0.45297274E-05
31	0.45505632D-02	0.20788450D-11	0.31628809E-03	0.90132809D 00	0.16500832D-10	0.45297274E-05
32	0.0	0.0	0.0	0.90132809D 00	0.13382565D-10	0.40586983E-05
33	0.41465759D-02	0.20788450D-11	0.34771326E-03	0.90547466D 00	0.13382565D-10	0.40586983E-05
34	0.0	0.0	0.0	0.90547466D 00	0.22737368D-10	0.52661562E-05
35	0.37079944D-02	0.20788450D-11	0.38062874E-03	0.90926266D 00	0.22737368D-10	0.52661562E-05
36	0.0	0.0	0.0	0.90926266D 00	0.17540255D-10	0.46060486E-05
37	0.34790039D-02	0.20788450D-11	0.41443459E-03	0.91274166D 00	0.17540255D-10	0.46060486E-05
38	0.0	0.0	0.0	0.91274166D 00	0.17540255D-10	0.45884926E-05
39	0.87258139D-01	0.17540255D-10	0.47946655E-04	0.10000000D 01	0.17540255D-10	0.45884926E-05
40						0.0

Fig. 4. *(Continued)*

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Monte Carlo
Simulation
Variance reduction

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)
This paper describes an algorithm and a FORTRAN subprogram, CHAIN, for simulating the behavior of an $(n+1)$ state Markov chain using a variance reducing technique called *rotation sampling*. The simulation of k *microreplications* is carried out in parallel at a mean cost $\leq O(\ln k)$ and with variances of sample quantities of interest $\leq O((\ln k)^2/k^2)$. The program allows for independent *macroreplications*, each of k microreplications, in order to facilitate estimation of the variances of sample quantities of interest. The paper describes theoretical results that underlie the algorithm and program in Section 1 and

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20. presents applications of interest for first passage time and steady-
state distributions in Section 2. Section 3 describes the algorithm
and CHAIN and an example in Section 4 illustrates how CHAIN works in
practice. Second 5 describes the options available for restarting
the simulation.

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